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Single-top t -channel hadroproduction in the four-flavour scheme with POWHEG and aMC@NLO

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ABSTRACT: We present results for the QCD next-to-leading order (NLO) calculation of single-top t -channel production in the 4-flavour scheme, interfaced to Parton Shower (PS) Monte Carlo programs according to the POWHEG and MC@NLO methods. Comparisons between the two methods, as well as with the corresponding process in the 5-flavour scheme are presented. For the first time results for typical kinematic distributions of the spectator- b jet are presented in an NLO+PS approach.

KEYWORDS: Hadronic Colliders, Monte Carlo Simulations, NLO Computations, QCD Phenomenology

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1 Introduction

Although experimentally challenging, the electroweak production of top (or antitop) quarks without their antiparticles, known as single-top production, is particularly important, not only because it provides a relatively clean place to study the electroweak properties of the top quark [1], but also because it allows for a direct measurement of V_{tb} [2, 3]. Moreover, single-top production is sensitive to many BSM models [4, 5], that in some cases are difficult to discover in other search channels. Single-top production is in general also a background for all searches where top-pair production and the production of a W boson in association with jets are an important background.

At leading order it is possible to classify the single-top hadroproduction mechanisms according to the virtuality of the W boson appearing in the tree-level diagrams: these mechanisms are known as s -, t -, and Wt -channel processes. The distinction becomes ill-defined at higher orders because of interference effects.¹ However, it makes sense to keep this nomenclature, since in general the kinematic properties of the final-state objects are very different when one includes higher-order corrections to s -, t - or Wt -channel Born-level processes. Moreover, preserving this distinction is also important because different BSM scenarios affect the three production mechanisms differently, making single-top studies a promising approach to distinguish among New-Physics models. Not surprisingly, experimental results and prospects for new analysis strategies at the Tevatron and LHC, as well as the aforementioned theoretical computations, are very often presented keeping this distinction. In this paper we will only concentrate on the main production mechanism, i.e. the t channel.

¹A notable exception is represented by the possibility of treating s and t channels separately when including QCD NLO corrections in the 5-flavour scheme (that will be shortly described later). The exact definition of the Wt channel is instead more complicated.

The theoretical effort to produce accurate predictions for this process is significant, and several improvements with respect to the first result of ref. [6] were achieved in the past: after the QCD NLO predictions obtained in refs. [7–9], studies on the impact of resummation [10, 11], off-shell effects [12, 13], and electroweak corrections [14] were also performed in recent years. All these results were based on the 5-flavour-scheme description of the process. In 2009 the first results for the NLO predictions in the 4-flavour scheme became available [15, 16]. More recently, factorizable NLO corrections to the top-quark decay process were computed and included in the MCFM framework [17], allowing for a consistent treatment of spin-correlation effects between the production and the decay stage, in the zero-width approximation for the top quark.

Single-top production is difficult to be observed as a signal itself, essentially because of the huge W +jets and the large $t\bar{t}$ backgrounds, which are hard to reduce by means of standard techniques, such as imposing cuts. As a consequence, to discriminate between signal and backgrounds and claim the evidence and the observation of single-top production, as well as to measure the s - and t -channel production rates, techniques based on neural networks, boosted decision trees and multi-variate analysis techniques were used at the Tevatron [18–21], and are currently employed at the LHC as well, on top of the cut-based ones [22–25]. Since all these strategies rely on the Monte-Carlo modelling of the signal and backgrounds, it is clear that the Monte-Carlo tools play a crucial role in understanding single-top production at hadron colliders. Therefore it is highly desirable to have event generators that consistently incorporate as much as possible of the improvements achieved in the theoretical predictions. An obvious but nontrivial direction to pursue is that of including QCD NLO corrections into Parton Shower (PS) Monte Carlo event generators. This has been achieved with the MC@NLO and the POWHEG methods [26, 27], so that nowadays it is possible to simulate with NLO+PS accuracy several processes relevant for lepton and hadron colliders, as well as deep-inelastic scattering. The recent automation of these techniques [28–32] allowed the simulation of processes with many external massless and massive partons and with non-trivial colour structures.

The simulation of s -, t -, and Wt -channel single-top production using the MC@NLO and the POWHEG methods is already possible, as described in refs. [33–36]. However, for the t -channel case, which was implemented following the 5-flavour scheme, there is some room for improvements. In particular, it is known that the modelling of the so called “spectator b ”, i.e. the hardest b jet not originating from the top-quark decay, is not very solid. The kinematic properties of this b -flavoured jet are, however, important to study single-top production in the t channel, since one usually requires one b jet with high and one with low transverse momentum (or, similarly, an anti- b tag) to tag a candidate single-top event as opposite to a $t\bar{t}$ pair, where typically two b jets with large momentum are present. For similar reasons, the kinematics of b -flavoured objects plays an important role in the discrimination between s - and t -channel processes. It is therefore desirable, especially for the precision that the LHC will achieve, to have tools as accurate as possible in describing these features.

To obtain NLO accuracy for the spectator- b observables in a NLO+PS program, a description of the single-top t -channel production process in the 4-flavour scheme [15, 16]

is required. The aim of this paper is to present results for the first implementation of this process in the `MCONLO` and `POWHEG` frameworks.

Let us elaborate on the differences and similarities between the 4- and 5-flavour schemes, whose corresponding representative leading-order Feynman diagrams are depicted in fig. 1.

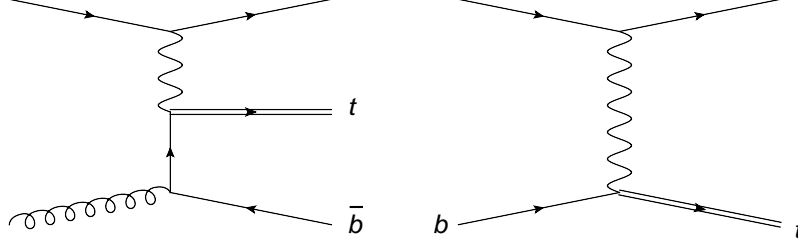


Figure 1. Representative leading-order Feynman diagrams for the single-top t -channel production in the 4- (left) and 5-flavour (right) scheme.

The difference is, in short, that in the former the PDF does not contain b quarks: all b quarks are generated in the matrix elements and cannot directly come from the (anti)proton. In the latter scheme, the description of the PDF contains the $g \rightarrow b\bar{b}$ splitting. This leads to the following considerations.

- In the 5-flavour scheme, the mass of the (initial-state) b quark has to be neglected in the matrix elements for factorisation to be valid. The cross section depends on the b mass (m_b) only through the starting scale for the evolution of the b quark in the PDF. On the other hand, in the 4-flavour scheme, the mass appears explicitly in the matrix elements, while the PDFs are independent of the b quark. In ref. [16] it has been shown that the b -mass dependence of the total cross section is similar in size in both schemes.
- In the 5-flavour scheme the PDF evolution resums logarithms of the form $\log(\mu_F^2/m_b^2)$, where μ_F is the factorisation scale, and the radiation thus resummed is described at leading-logarithmic accuracy. The clear advantage is that due to the resummation the total rate can be predicted precisely. In the 4-flavour scheme, these logarithms are not resummed. However, the non-logarithmic contributions to the $g \rightarrow b\bar{b}$ splitting are already taken into account in the LO description of the process, which leads to a more precise prediction of the b -quark distributions than in the 5-flavour scheme. When including NLO corrections in the 4-flavour scheme, the first logarithms are included as well. Similarly, at the NLO level in the 5-flavour scheme, also the first non-logarithmic contributions due to radiation are correctly accounted for.
- The running of the strong coupling α_s depends on the number of flavours.

The $m_b = 0$ approximation in the 5-flavour scheme can be improved systematically by replacing (higher-order) contributions that have no b quarks in the initial state, by

corresponding contributions in which $m_b \neq 0$. With this improvement the 4- and 5-flavour-scheme descriptions become exactly equivalent when all orders in perturbation theory are included.

In refs. [15, 16] it was shown that with a proper physically-motivated choice of factorisation and renormalisation scales, the agreement of the two approaches is good already at the NLO approximation. Therefore, the 4-flavour-scheme calculation, which has the obvious advantage of a more precise treatment of the spectator- b quark, is the preferred one for an exclusive description of the process. This statement is confirmed by the conclusions of ref. [37], where the issue of choosing a 4- or a 5-flavour scheme for key processes at hadron colliders, including single-top, is addressed. There it is indeed shown that the size of the initial-state logarithms, $\log(Q^2/m_b^2)$, that are resummed in the b PDF within the 5-flavour scheme is modest, except at large Bjorken x 's. Moreover, the effective scale Q^2 that enters these logarithms is typically smaller than the hard scale of the process, being accompanied by universal phase-space suppression factors, which further reduces the size of these logarithms.

This paper is organised as follows. In sec. 2 we briefly describe some technicalities of the computer programs used to obtain the results presented in the following. In sec. 3 we show typical distributions relevant for single-top studies, comparing the pure-NLO results with those obtained with our NLO+PS codes. We compare different prescriptions for the matching (POWHEG vs MC@NLO) as well as different showering models (PYTHIA vs HERWIG). Scale dependence and PDF errors are displayed for the results obtained with aMC@NLO, while a full study encompassing all other sources of uncertainty, *e.g.* the values used for the b - and the top-quark masses, is beyond the scope of this work and has not been attempted. Instead, we perform a comparison with the results obtained in the 5-flavour scheme, in particular for the spectator- b jet. Finally, in sec. 4 we give our conclusions.

2 Description of the implementation

To simulate the 4-flavour single-top t -channel production with NLO+PS accuracy, the POWHEG BOX package [28] and the aMC@NLO framework [29] have been used. In this section we shortly discuss the technical aspects of the codes employed to obtain the results presented in this work.

The aMC@NLO code is a tool to compute processes at NLO accuracy matched to parton showers using the MC@NLO method [26]. It is completely automatic and general, its only limitation being represented by CPU availability. It is built upon the MadFKS [38] framework which uses the FKS subtraction scheme [39] to factor out the poles in the phase-space integration of the real-emission squared amplitudes. In this work, we do not use MadLoop [40] to evaluate the virtual corrections, and exploit the analytic results of ref. [15] instead.

The POWHEG BOX is a program that automates all the steps described in ref. [41], turning a NLO calculation into a POWHEG simulation. The details of how the program works have been largely described in ref. [28], and therefore will not be repeated here. To implement the NLO computation in the POWHEG BOX program, we obtained the needed inputs as follows.

- The Born kinematics was obtained mapping the $2 \rightarrow 3$ phase space to a multidimensional hypercube where the random numbers are generated. We have built the phase space using the Bycling-Kajantie [42] parameterisation.
- The tree-level $2 \rightarrow 3$ and $2 \rightarrow 4$ matrix elements were obtained using `MadGraph4` [43].
- The same virtual corrections as computed in ref. [15] (and implemented in the `MCFM` package) have been used here as well. We have also checked the numerical value for the Born and the 1-loop finite part against the value in Appendix 2.8 of ref. [40].
- Although at the Born level there are 5 coloured partons, the colour-linked squared amplitudes for this process factorise the full Born squared amplitudes: no colour correlation is possible between the light and the heavy current, since a W boson is exchanged. For the same reason, the assignment of planar colour connections to the $2 \rightarrow 3$ processes is trivial.
- The spin-correlated squared amplitudes were computed using `FeynCalc` [44], and checked by comparison with the collinear limits of the corresponding $2 \rightarrow 4$ radiative corrections.

The complete NLO implementation has also been extensively checked with the implementation available in `MCFM`, which makes use of the Catani-Seymour subtraction scheme [45]. Agreement was found for total rates and for several distributions.

3 Results

In this section we present our results at different levels of sophistication, comparing the fixed-order partonic predictions with those after the showering and the hadronisation stage. We will show only results for top production at the Tevatron and at the LHC (with hadronic center-of-mass energy $\sqrt{S} = 8$ TeV), although the generation of anti-top events was also implemented and tested, leading to similar results as those presented here. At the matrix-element level the top quarks have been assumed to be stable: the decays have been generated by the Shower Monte Carlo programs and forced to be semi-leptonic ($t \rightarrow b \ell^+ \nu$). Branching ratios have been set to 1, so that plots are normalised to the total cross section.

We have chosen renormalisation and factorisation scales following the arguments presented in ref. [15]: the scale for this process is not determined by the heavy top quark, but rather by the (maximal) transverse momentum of the b quark. We have therefore opted for

$$\mu_R = \mu_F = 4\sqrt{(m_b^2 + p_{T,b}^2)} \quad (3.1)$$

as our central scale choice.² We have also checked that the choice in (3.1) is numerically close to the scale $Q(z)$ proposed in ref. [37] in the kinematic range relevant for the results

²In refs. [15, 16] the scale choices for the heavy- and light-quark lines were different ($\mu_h = m_t/4$ and $\mu_l = m_t/2$, respectively) and it was found that the total scale dependence is dominated by that coming from the heavy-quark line. We have therefore opted for a scale based on the kinematics of the heavy-quark line, which reflects the properties of the spectator- b quark better than a fixed scale. We expect that the

presented in the following. For the POWHEG results, the b -quark momentum is understood to be taken at the underlying-Born level. We have used the MSTW2008(n)lo68cl_nf4 sets [46] of parton-distribution functions for the (N)LO predictions (and the corresponding sets for the 5-flavour results presented in sec. 3.3), with default values and running of α_s as given by the LHAPDF [47] interface.

The values of physical parameters entering the computation are as follows:

$$\begin{aligned} m_t &= 172.5 \text{ GeV}, & m_b &= 4.75 \text{ GeV}, & m_W &= 80.398 \text{ GeV}, \\ \alpha^{-1} &= 132.338, & \sin^2 \theta_W &= 0.22265, \end{aligned}$$

and a diagonal CKM matrix has been employed.

Jets have been defined according to the inclusive k_T algorithm [48], as implemented in the FastJet package [49, 50], setting $R = 0.7$ and imposing a 20 (30) GeV lower cut on jet transverse momenta for the Tevatron (LHC). Moreover, jets are required to have pseudorapidity $|\eta_j| < 2.5$. The jets containing at least one b -flavoured particle (a b quark at the parton level, one or more B hadrons for showered results) are called “ b -flavoured jets”, as opposite to the others, denoted “light jets”.

We have run HERWIG 6.520 [51] and PYTHIA 6.4.22 [52] with default parameters (i.e. without using a particular tune), and with multiple-parton interactions and underlying event switched off. PYTHIA has been run with the p_T -ordered shower. To simplify the analysis, we have set the lighter B hadrons, the muons, and the pions stable.

In order to estimate PDF and scale dependence for the aMC@NLO results, we have used the reweighting method described in ref. [53], which allows the extraction of these theoretical uncertainties without any extra CPU costs. For the PDF dependence the events are reweighted by the 2×20 MSTW2008 error sets, whereas for scale variations the events obtained with the scales in (3.1) are reweighted by the following six combinations, $(\mu_F, \mu_R) \times \{(1/2, 1/2), (1/2, 1), (1, 1/2), (2, 1), (1, 2), (2, 2)\}$, and the envelope of the distributions constitutes the uncertainty band.

The results in figs. 2-7 are characterised by the following pattern. In the main plot there are three curves corresponding to aMC@NLO+HERWIG (black solid), POWHEG+HERWIG (blue dashed) and POWHEG+PYTHIA (red dotted). In the upper inset the relative scale (red dotted) and PDF (black dashed) uncertainties for the aMC@NLO+HERWIG results are shown. In the lower inset the ratio of the aMC@NLO (black solid), POWHEG+PYTHIA (red dashed), standalone HERWIG (blue dotted) and the fixed NLO (green dot-dashed), over the POWHEG+HERWIG results are presented. The standalone-HERWIG result has been obtained showering events generated according to their LO cross section.

3.1 Tevatron results

In figs. 2 and 3 we show the transverse momentum and the rapidity of the top quark and of the hardest light jet, respectively. As expected, a very good agreement is observed between

results presented here give a better description with respect to refs. [15, 16] when the spectator- b quark has a large transverse momentum, and that no other observables are hampered, because $4\sqrt{(m_b^2 + p_{T,b}^2)} \sim m_t/4$ for the bulk of the events.

the NLO and the NLO+PS results. In particular, all the simulations that include NLO corrections show an excellent agreement for observables related to the top-quark kinematics. This is slightly less the case for the hardest light jet (see, for instance, the right plot of fig. 3), even though the effect is still well within the uncertainty band (here shown only for the aMC@NLO results): differences of the size of those appearing in fig. 3 are however to be expected for observables affected by extra radiation. Conversely, the discrepancy with the LO+PS curve is larger, since in the 4-flavour scheme the NLO corrections are non-negligible, as noticed in ref. [15]. Theoretical uncertainties, dominated by scale dependence, are in general of the order of $\pm 10\%$ and constant for the observables here considered, with the exception of an increase to $\pm 20\%$ for the top rapidity at large and negative values, due to the gluon-PDF uncertainty at large Bjorken x 's.

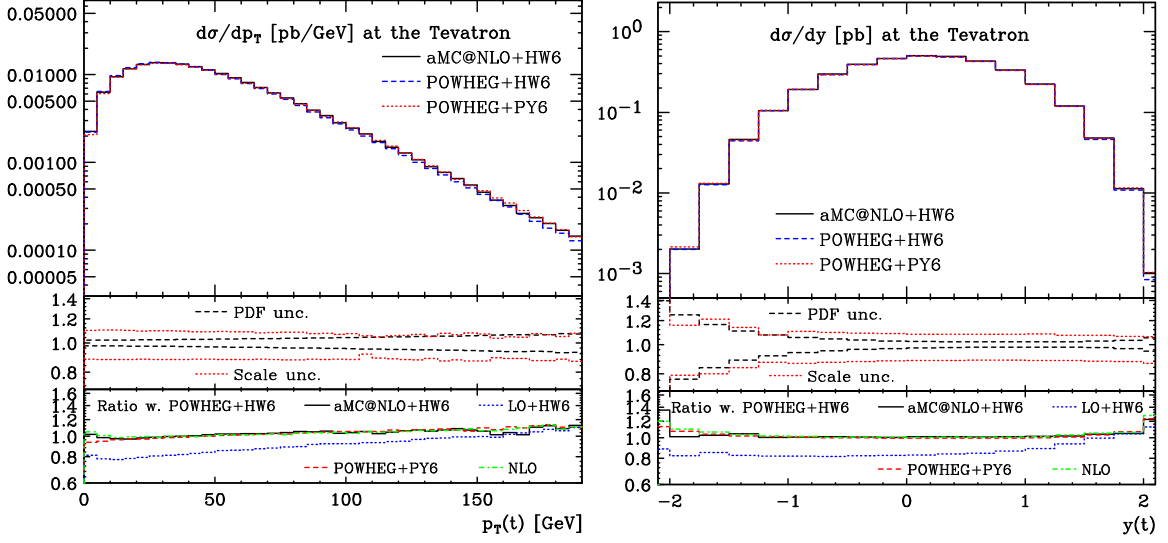


Figure 2. Transverse-momentum and rapidity distributions of the top quark at the Tevatron.

In fig. 4 the transverse momentum and the rapidity of the second-hardest b jet are shown. As mentioned in the previous sections, a good understanding of the b -jet kinematics is very important to discriminate between single-top and $t\bar{t}$ events. In particular, the typical single-top signature is the presence of a hard and central b jet from the top decay and of a second b jet (the spectator- b jet) with larger rapidity and moderate p_T , arising from the initial-state $g \rightarrow b\bar{b}$ splitting, as opposite to $t\bar{t}$ events where typically two hard and central b jets are present.

In our simulations, top-quark decays are not included at the matrix-element level, therefore we have omitted the fixed-order results from these plots, as a comparison with showered predictions would not be fair: in fact, for the latter the second-hardest b jet is mostly the spectator- b jet, contaminated by jets coming from the top decay, while at the parton level there is no second-hardest b jet, and the spectator- b jet is always the hardest.

For NLO+PS predictions, transverse momenta are in good agreement with each other, whereas the aMC@NLO rapidity distribution is slightly broader than the ones obtained with

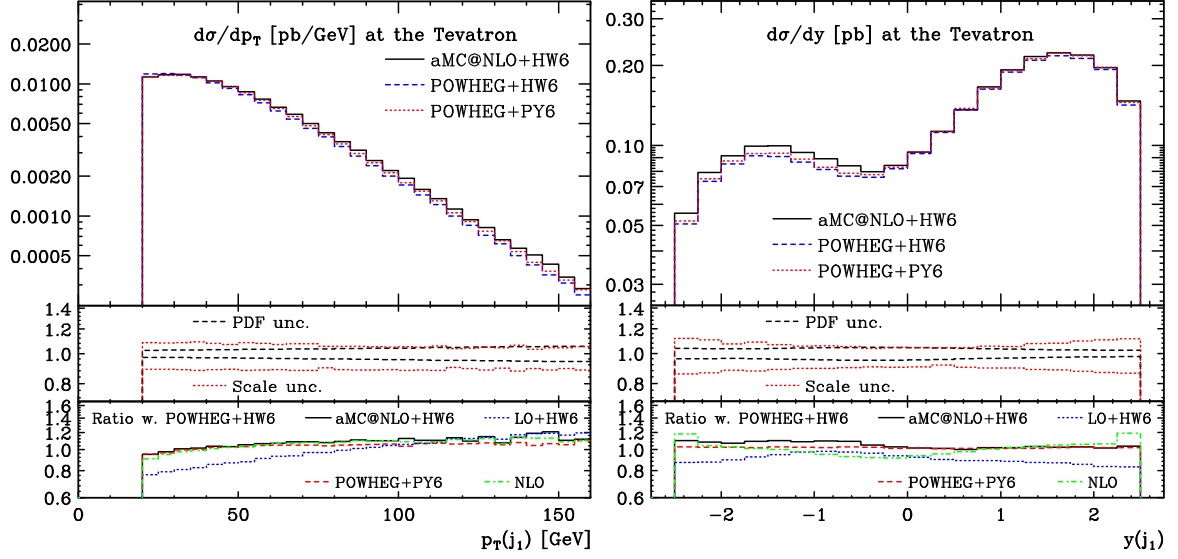


Figure 3. Transverse-momentum and rapidity distributions of the hardest light jet at the Tevatron.

POWHEG. However, as the theoretical-uncertainty bands, here of the order of $\pm 15\%$, are included, the aMC@NLO and the POWHEG results become compatible. Residual discrepancies at this level should be considered as an estimate of the systematic uncertainty arising from the use of different NLO+PS-matching methods.

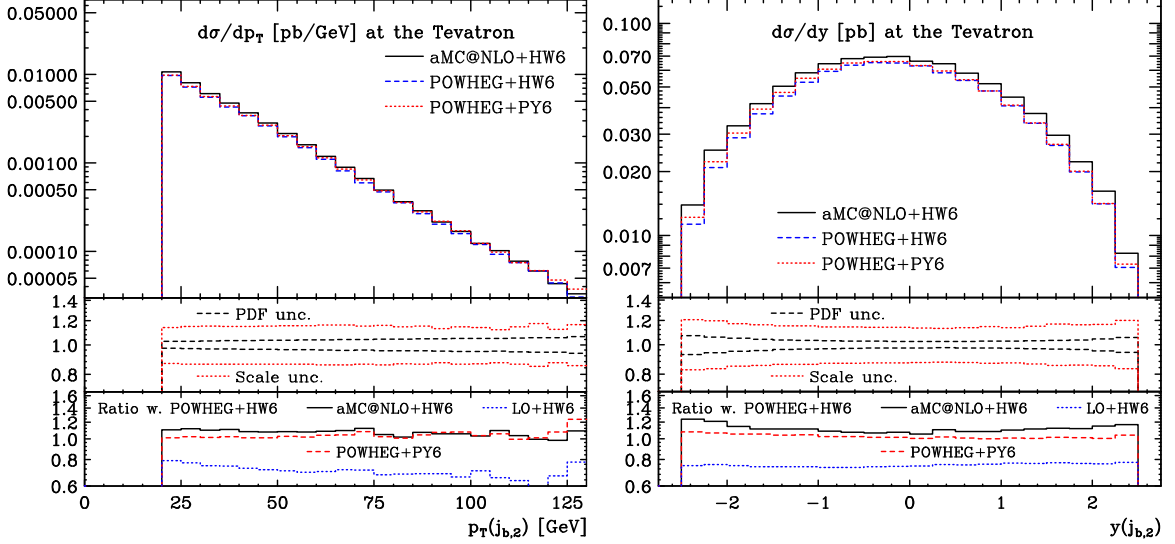


Figure 4. Transverse-momentum and rapidity distributions of the second-hardest b jet at the Tevatron.

3.2 LHC results

In figs. 5-7, the same observables as in figs. 2-4 are shown for single-top production at the LHC, with a center-of-mass energy of 8 TeV. Considerations similar to the above ones can be drawn by inspecting these plots. One can notice some more pronounced differences between the aMC@NLO and the POWHEG results for the light jet. These are the only observables where the disagreement between the two predictions exceeds the theoretical-uncertainty bands. In particular, the aMC@NLO result is larger, and although the enhancement is essentially uniform over the rapidity range examined (right plot of fig. 6), a shape difference with respect to the two POWHEG predictions can be seen in the p_T spectrum (left plot of fig. 6). However this observable, in the phase-space region considered, is sensitive to the behaviour of the parton shower in its first emission: therefore the aMC@NLO result closely follows the shape of the HERWIG one, while POWHEG is closer to the fixed-order NLO. As commented before, in experimental analyses, these differences should be considered as a theoretical systematics of the NLO+PS-matching scheme. Scale and PDF variations are smaller than for the Tevatron, and in general constant and of the order of $\pm 5\%$ for top- and hardest-jet-related observables, and $\pm 10\%$ for the spectator- b jet.

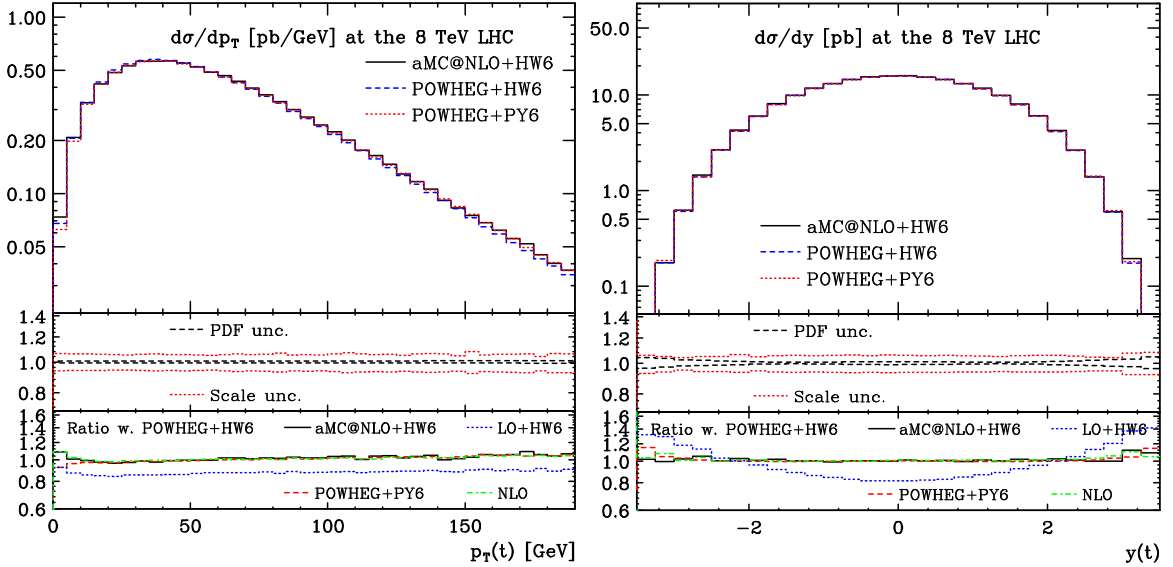


Figure 5. Transverse-momentum and rapidity distributions of the top quark at the LHC.

As a final comment, we notice a remarkably good agreement between the POWHEG predictions obtained with the PYTHIA and the HERWIG shower, for all the observables considered, both at the Tevatron and at the LHC. It is therefore unlikely that truncated showers be relevant in order to simulate with NLO+PS accuracy the single-top t -channel process in the 4-flavour scheme. The residual, very small dependence on the shower model employed can be considered as a systematic effect intrinsic in the POWHEG simulations.

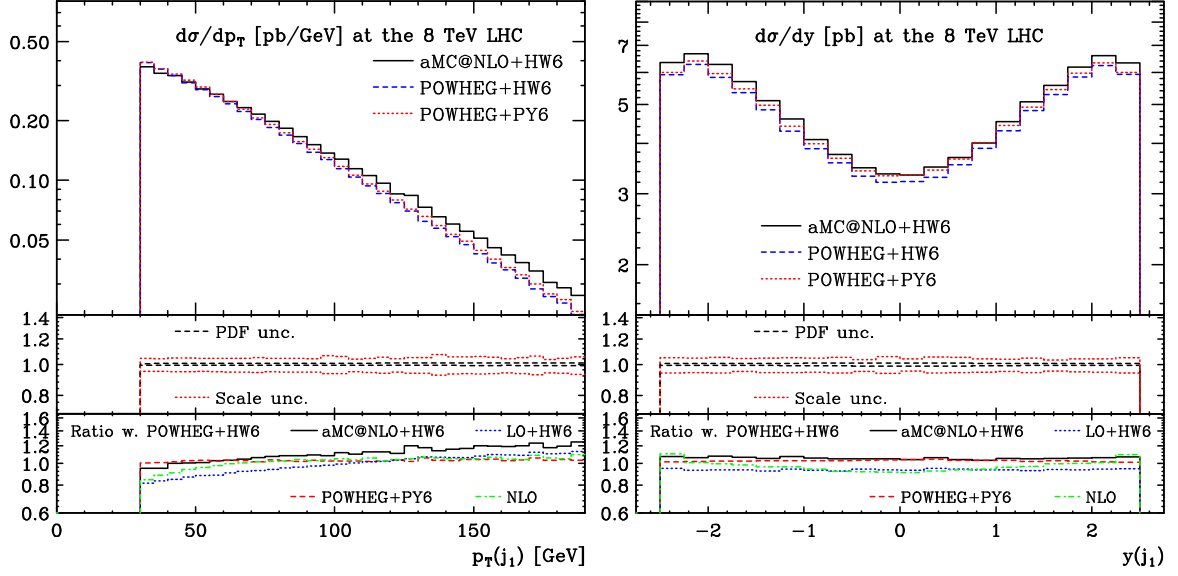


Figure 6. Transverse-momentum and rapidity distributions of the hardest light jet at the LHC.

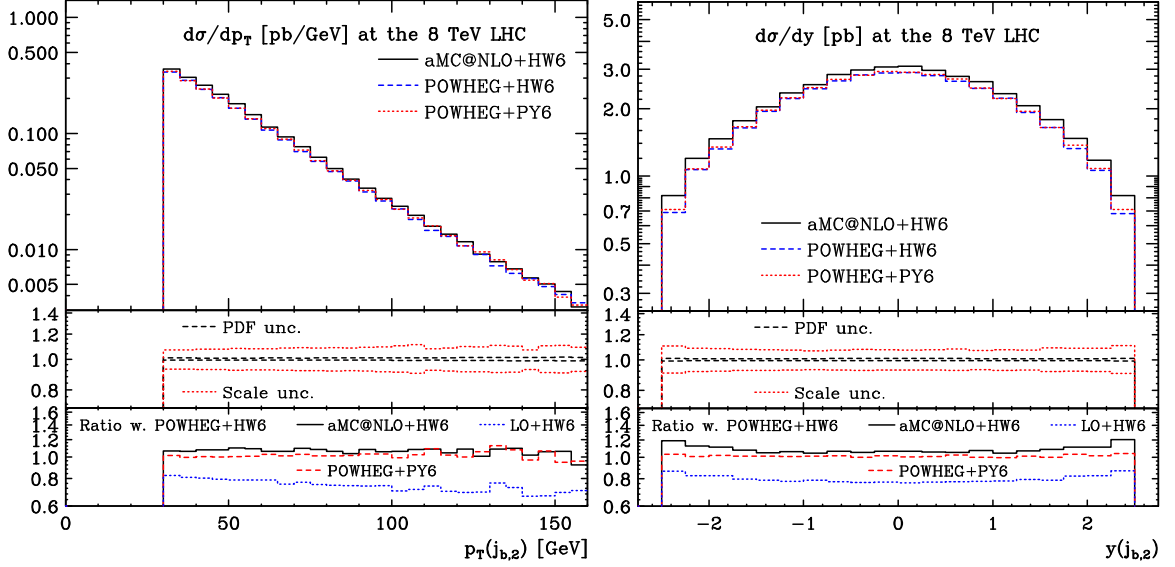


Figure 7. Transverse-momentum and rapidity distributions of the second-hardest b jet at the LHC.

3.3 Comparison between the 4- and the 5-flavour MC simulations

In this section we want to briefly comment on the robustness of the NLO+PS simulation of t -channel single-top in the 5-flavour scheme, and compare it with the new implementation presented in this paper. As mentioned in the introduction, from a perturbative point of view the 4- and the (improved) 5-flavour schemes are exactly equivalent only if all orders in perturbation theory are included, even though, as shown in refs.[15, 16], the agreement

is good already at the NLO level. In the following, we would like to confirm this for the NLO+PS results.

It is known [35, 54] that in the simulation of single-top in the 5-flavour scheme, distributions involving b -flavoured objects coming from a $g \rightarrow b\bar{b}$ initial-state splitting show unphysical pathologies at low p_T and high rapidity, when the HERWIG shower is used. The reason for this is a simplified treatment of the non-perturbative corrections, in particular due to a mismatch between the scale at which the backwards shower evolution is switched off and the one at which the b quarks in the PDF are switched on. In this respect, it is also worth recalling that when the NLO+PS matching is performed with MC@NLO using the Herwig++ event generator, the unphysical spikes at large y_b disappear, as it was shown in [54]. It is clear that in the 4-flavour approach the potential mismodelling of the B -hadron kinematics is fixed, because there is no initial-state b quark at the matrix-element level. Therefore we expect the NLO+PS predictions obtained in the 4-flavour scheme to be very solid when observables related to the spectator- b jet (arising from the B hadron, originated in turn by the \bar{b} quark) are considered. In fig. 8 we show the acceptance for the spectator- b

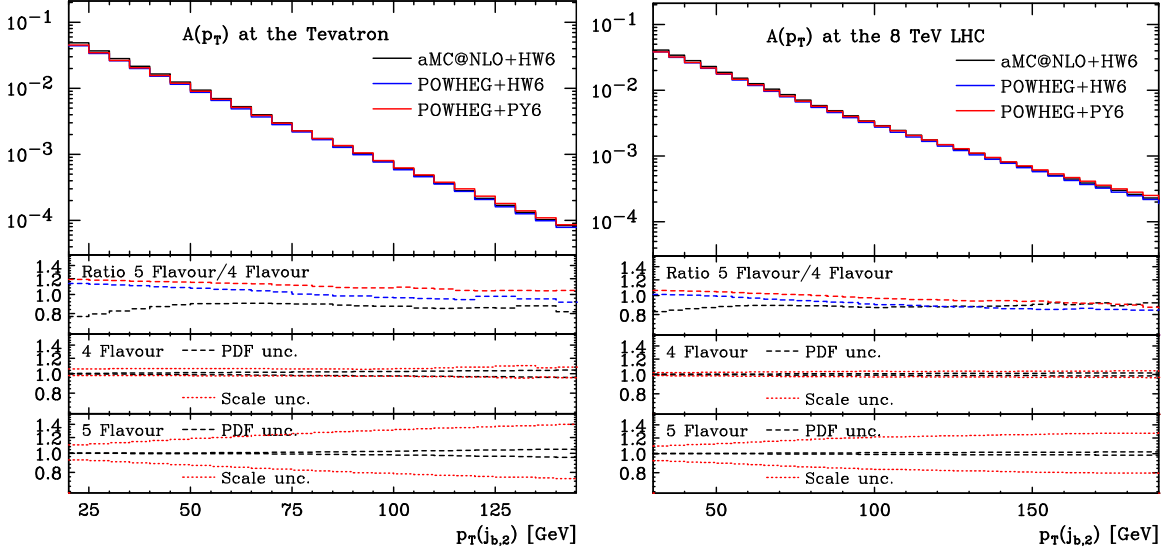


Figure 8. Acceptance as a function of the second-hardest b -jet transverse momentum, as defined in eq. (3.2).

jet (identified as above with the second-hardest b jet). The acceptance is defined as

$$A(p_T) = \frac{1}{\sigma_{\text{tot}}} \int_{p_T}^{\infty} dp_T^{(j_{b,2})} \frac{d\sigma}{dp_T^{(j_{b,2})}}, \quad (3.2)$$

where σ_{tot} is the total NLO inclusive cross section, and jets are required to have $|\eta_j| < 2.5$. In the main panels of both plots, the NLO+PS results obtained in the 4-flavour scheme are shown. In the upper insets we show the ratio between the NLO+PS acceptances computed with the 5- and the 4-flavour scheme, whereas in the middle and lower insets the theoretical

uncertainty for this observable is reported, as computed with **aMC@NLO**, using the 4- and the 5-flavour scheme, respectively.³

First of all, we notice in the main panels that the **aMC@NLO** and the two **POWHEG** results are practically indistinguishable. This is encouraging, since those for observables related to the spectator- b jet are genuinely NLO-accurate predictions in the 4-flavour scheme, and therefore we expect the generators to produce results very close to each other. In the upper insets we observe 10-15% deviations from 1 in the ratio between the 5- and the 4-flavour predictions. More precisely, ratios are close to 1 at the LHC in the whole p_T range, whereas differences are more pronounced at the Tevatron, and slightly more evident for the **aMC@NLO** results. The smaller discrepancy at the LHC is compatible with the observations of ref. [37], since the Bjorken x 's relevant to collisions at the LHC are on average smaller than those at the Tevatron, which suppresses the logarithmic contributions that are resummed by the b PDF in the 5-flavour but not in the 4-flavour total rates. However, the impact of these logarithms is quite moderate and, when theoretical uncertainties are taken into account, the 4- and 5-flavour results are compatible with each other in most of the p_T range: the uncertainty of the 5-flavour prediction is indeed sizable (especially at the Tevatron), as can be seen in the lower insets, since acceptances have LO accuracy when computed in this scheme. In particular, the increase in the uncertainty at high transverse momentum is what is expected in the 5-flavour scheme for this observable, strictly related to the p_T of the Born system, as discussed in [53, 55]. The 4-flavour prediction itself is instead much more accurate, as can be evinced from the middle insets.

At low transverse momentum, however, the **aMC@NLO** ratios deviate significantly from 1 and from the **POWHEG** results, as is evident looking at the upper insets. This behaviour is caused by the 5-flavour prediction, and it is understood as arising from the different way in which the two programs handle the $g \rightarrow b\bar{b}$ initial-state splitting. In particular, in the region of low $p_T^{(j_{b,2})}$, **aMC@NLO** entirely relies on the underlying-shower description of the kinematics, thus inheriting the above-mentioned unphysical **HERWIG** feature in the treatment of the spectator b . Conversely, **POWHEG** performs the hardest emission in a way independent of the parton shower it is interfaced to, which partially prevents its predictions from this mismodelling. This interpretation is sustained by the closeness of the two **POWHEG** curves in the upper insets.

From this comparison, one can conclude that the 4-flavour and the 5-flavour approaches are both reliable (barred a well-known **HERWIG** unphysical behaviour) and in mutual agreement when theoretical uncertainties are taken into account, although, as expected, the predictions obtained in the 4-flavour scheme are more precise, containing NLO corrections, and more solid than the 5-flavour ones.

4 Conclusions

In this article we have presented for the first time two independent computations of single-top production in the t channel using the 4-flavour scheme, matching the QCD next-to-

³For the 5-flavour predictions we have used the top mass as the central value for renormalisation and factorisation scales, and the **MSTW2008nlo** PDF set.

leading-order corrections to parton showers. We have used the POWHEG and the MC@NLO prescriptions, as implemented in the automated frameworks POWHEG BOX and aMC@NLO.

We have studied observables typically considered in experimental analyses, and compared the two NLO+PS predictions with each other as well as with fixed-order results. We have generally found very good agreement for inclusive observables, and also for observables more sensitive to QCD emissions, such as the light-jet and the spectator b -jet transverse momenta and rapidities. In general the predictions are compatible when theoretical uncertainties are taken into account, and the small differences encountered can be ascribed to systematic effects of the choice of different matching frameworks. We conclude therefore that the POWHEG and MC@NLO results are consistent, and so are the two predictions obtained by matching POWHEG with the PYTHIA and the HERWIG shower.

We have also compared NLO+PS predictions obtained in the 4- and in the 5-flavour schemes. It is known that NLO+PS results obtained in the latter scheme can exhibit unphysical features in the description of the b -flavoured particle produced in the fragmentation of the b quark coming from the hard process. The kinematics of this particle needs to be predicted reliably, being relevant for the description of the spectator- b jet typically arising from it, which in turn is important in experimental analyses. We have computed the acceptance as a function of the spectator b -jet transverse momentum in both schemes. The 4-flavour results are the first NLO+PS-accurate predictions for this observable, and show an excellent agreement between the POWHEG and aMC@NLO implementations. The differences between 4- and 5-flavour scheme, in the region unaffected by the initial- b HERWIG mismodelling, are small for the acceptance, and within the theoretical uncertainty. The latter is dominated by the large error affecting the 5-flavour result, which is only LO-accurate for this observable; the 4-flavour prediction contains instead NLO corrections, and is therefore more accurate, as we have shown explicitly.

The implementations described in this publication and/or the event files used to produce the distributions shown here are publicly available in the POWHEG BOX repository and on the aMC@NLO webpage. The spin correlations between the production and the decay of the top quark can be included as well, which is left for future work.

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